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Three-Dimensional Flow Modeling of a Self-Wiping Corotating Twin-Screw Extruder. Part II: The Kneading Section

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Three-dimensional flow simulations of kneading elements in an intermeshing corotating twin-screw extruder are performed by solving the Navier Stokes equations with a finite element package, Sepran. Instead of using the whole geometry of the 8-shaped barrel a simplified geometry is used, representing a large part of the geometry during the rotating action of the kneading paddle. The goal of these calculations is to study the dependence of several factors that influence mixing, such as shear rate, elongation rate, pressure, and the flow profile in the extruder on various extruder parameters, such as fluid viscosity, rotation speed, and throughput.

The shear and elongation rate and the pressure drop are calculated for varying viscosities. The various stagger angles possible for disc configurations in the corotating twin-screw extruder are modeled. The axial backflow volume is calculated for varying values of rotation speed and throughput.

INTRODUCTION

Calculations of the flow profile in kneading elements in the intermeshing corotating twin-screw extruder have been done by Yang *et al.* (1). They show that the geometry of the volume, in which the fluid flows, changes during the rotation of the screw, as is described in the section on **Geometry and Mesh**. Here a three-dimensional modeling of the flow profile in the kneading section of the intermeshing corotating twin-screw extruder is performed. By far the majority of the studies on the modeling of the twin-screw extruder have concentrated on 2D or quasi-3D modeling of the flow in the transport section in extruders (1–3).

In the intermeshing twin-screw extruder, one screw wipes its mate and vice versa. The self-wiping action makes the twin-screw extruder attractive for handling many polymers. It eliminates dead spots where polymer can collect, stagnate, and degrade (4). In the

kneading section the material flows from one element to the next. Usually the co-rotating twin-screw equipment comprises a housing (called the barrel) and two identical parallel shafts equipped with identical screw or paddle elements. The number of tips of the paddles can be chosen, but the cross section of a paddle with 1, 2, 3, or 4 tips must meet certain design specifications. These are well known, and much work has been done by Booy (4) on the geometrical constraints of corotating extruders.

The geometry of the kneading element in this work is shown in Fig. 1. The computational mesh used (Fig. 1b) is part of the geometry as found in the corotating twin-screw extruder in Fig. 1a. The geometry will be described in more detail under **Geometry and Mesh**. The 3D flow profile is calculated with the boundary conditions given under **Boundary Conditions**.

A number of assumptions will be made:

- The flow is laminar, isothermal, and stationary.
- The fluid is incompressible, Newtonian and, where relevant, has a viscosity of 100 (Pas). Although the

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Fig. 1a. The cross section of the geometry in the kneading section. Fig. 1b. The geometry of part of the channel in the kneading section as used in the computation, the stagger angle is 90°. Fig. 1c. Cross-sectional mesh when the stagger angle is 60°.

Newtonian model is an obvious simplification for many situations occurring in practice, it is expected to provide a valuable first insight into the flow phenomena. Non-Newtonian fluid behavior will be incorporated in our future work.

- The element is completely filled.
- The outflow profile of an element is transformed into the inflow profile of the next element.

The backflow volume is an important parameter for mixing, and it is computed by integration of the axial (down channel) velocities over the part of the cross section where these velocities are negative. The pressure difference is dealt with under **Results**. The shape of the flow profile, the backflow volume, the shear- and elongation rate are calculated. The elongation and shear rate are defined under **Results**. In this work, within the limitations of the calculations, results are obtained for the shear and elongation rate as a function of rotation speed and throughput.

MATHEMATICAL METHOD

As mentioned before, the simulation is based on a stationary model. The equations to be solved are those for isothermal laminar flow of a Newtonian, incompressible fluid without body forces:

conservation of mass:

$$\text{div } \vec{v} = 0 \quad (1)$$

conservation of momentum:

$$\rho(\vec{v} \cdot \nabla)\vec{v} + \nabla p = \text{div } t \quad (2)$$

where p denotes the pressure, ρ the density, $\vec{v}$ the velocity, and t is the Newtonian fluid stress tensor

given by:

$$t = \eta(\nabla \vec{v} + \nabla \vec{v}^T) \quad (3)$$

where η is the viscosity. Equations 1 and 2 are discretized. The Penalty method, described by Cuvelier *et al.* (5), is used for the discretization of the incompressibility constraint. The continuity equation is adapted by adding a small term containing the pressure:

$$\epsilon p + \text{div } \vec{v} = 0 \quad \epsilon: \text{small} \quad (4)$$

By this method the pressure, p , is eliminated from the momentum equation. The velocity and pressure are then separated. The equations, after discretization by Galerkin's method, are:

$$S\vec{u} - N(\vec{u})\vec{u} - (1/\epsilon)L^T M_p^{-1} L\vec{u} = 0 \quad (5)$$

$$\vec{p} = - (1/\epsilon)M_p^{-1} L\vec{u}$$

where S is the stress matrix, $\vec{u}$ the vector of the unknown velocity values, $N(\vec{u})\vec{u}$ the discretization of the convective terms, L the divergence matrix, M_p the pressure mass matrix and $\vec{p}$ the vector of the unknown pressure values. In the numerical solution, the non-linear terms in Eqs 4 and 5 are linearized with the Picard linearization and Newton iteration. In the solutions to the 3D Navier Stokes equations a triquadratic isoparametric brick element is used. The velocity is approximated by a full triquadratic approximation based on the 27 nodes from an element. The pressure is approximated linearly and is discontinuous.

The numerical error in the velocity results decreases quadratically with the mesh size, but the results for the pressure are only first-order accurate [see Cuvelier *et al.* (5)]. However, the finite-element mesh used in our computations has been chosen sufficiently fine to guarantee satisfactory overall accuracy. We emphasize that the Penalty function method allows the extruder throughput to be prescribed, whereas the required pressure drop follows from the computations.

DEFINITION OF THE PROBLEM

Geometry and Mesh

During one rotation the geometry of the volume in the kneading section changes, as shown in Fig. 1a. Changing the geometry and boundary conditions at every time step in the calculations would be too time consuming for a fully three-dimensional modeling. However, in Fig. 1a it can be seen that part of the geometry remains the same during a large part of the rotation. The geometry that is used in these calculations is based on equations given by Booy (4), and shown in Fig. 1b. In order to obtain convenient boundary conditions a new coordinate system is chosen. In the geometry in Fig. 1b the screw is at rest while the barrel wall moves. The geometric parameters used in Booy's equations (4) are C_i and R_s , where C_i (40 mm) is the distance between both axes of the screws and R_s

(25 mm) is the radius of the screw. The kneading elements have a width of 14 mm.

There are several possibilities to position a second "paddle" behind the first paddle. The computational mesh shown in Fig. 1b refers to the case with stagger angle 90° , the one of Fig. 1c to the 60° case. In these Figures both the part of the plane that is blocked in the inflow plane and the part of the plane that is blocked in the outflow plane can be distinguished. The stagger angle is defined as the angle between two consecutive screw elements and is taken in the same direction as the rotation of the screw.

Boundary Conditions

The boundary conditions are as follows: on the screw a zero velocity, on the barrel a tangential velocity according to the rotation speed with a zero axial velocity (both owing to the no-slip condition).

On the inflow plane of the first kneading element we prescribe a uniform axial velocity for the entire region. Part of the outflow plane is blocked because of the second screw element, as shown in Fig. 2, for the case of a 90° stagger angle. In the nonblocked parts of the outflow plane no velocity is prescribed, but a free stress boundary condition is imposed instead. The inflow plane of the second element is partially blocked by the first element (calculations are done for successive elements). The inflow velocities to be prescribed in the two nonblocked areas follow from the transfer of the outflow profile of the previous element, as indicated in Fig. 2. The boundary conditions on the outflow plane are the same as those for the previous

element. In this way an arbitrary number of kneading elements can be joined together.

The Reynolds number values used are small ($Re \cong 0.04$). The materials usually processed in the corotating twin-screw extruder are polymers with high viscosity. The viscosities vary, since during processing the polymers have changed, because of temperature differences. Because the flow is assumed to be isother-

Fig. 2. The transformation of the outflow profile to the inflow plane of the next element.

Fig. 3. Development of the flow profile along the kneading element, stagger angle 90° , $N = 100$ rpm, $Q = 80$ ml/s. Bottom picture: first element, top picture: second element.

mal, the viscosity is assumed constant in the kneading element. However it is possible to change the viscosity in the next kneading element, which is of interest since the viscosity might influence the flow profile in the extruder (see **The Influence of the Viscosity on the Flow**).

RESULTS

First the symmetrical case with a stagger angle of 90° between the kneading elements is considered (Fig. 1b). Calculations are performed for several rotation speeds, throughputs, and viscosities, as defined in the previous section. The equations, given to fit the graphs, represent the results within 5% (mean values are always calculated for the second element).

The Axial Velocities

In Fig. 3 axial velocity profiles in the first and the second kneading element are shown at five axial positions along the kneading element. A flat profile is assumed at the inflow plane of the first element. The left part of the outflow profile enters the right part of the inflow plane of the next element because of the angle of 90° between the second and first kneading element. From this Figure it is clear that (for the first element) the inflow profile is different from the outflow profile. The main tendency for the outflow profile is to develop a negative outflow (backflow) at one side of the outflow plane. The prescribed barrel velocity draws the fluid to the left while the throughput is in the axial direction. If the barrel velocity is sufficiently large compared with the incoming velocity, the resulting axial velocity on the left is larger than the mean axial velocity in the inflow plane. Integration of the axial velocity in the outflow plane must produce the throughput entering the inflow plane, leading to a deficit of fluid created on the right-hand side of the kneading volume. This deficit has to be filled again, so fluid has to flow to this spot. The flow created in this

way is the backflow. This name is chosen since the kneading element sucks the fluid back from the next element.

It is found that the outflow profile of the first and the second kneading element have almost the same shape. From this it is concluded that the profile that develops over the axial length of the first kneading element, as shown in Fig. 3, is established.

The Axial Backflow Volume

To characterize the flow profile, the backflow volume will be used as a measure of the influence of the various extruder parameters on the flow profile. The backflow volume is calculated at a number of axial positions along the kneading element, by integration of the negative axial velocities in the transverse plane. The graph in Fig. 4 shows the absolute backflow, $|Q_b|$, when eight kneading elements are placed in series. The maximum values always appear at the outflow plane that coincides with the inflow plane of the next element.

Figure 5 shows that the axial backflow volume through the outflow plane of the second kneading element increases with increasing rotation speed. A decrease of the backflow with increasing throughput is found. The lines in Fig. 5 are fitted with:

$$|Q_b| = 0.06223 \cdot N \cdot \exp(-4.8176 \times 10^{-3} \cdot Q) \quad (\text{ml/s}) \quad (6)$$

Q_b : (ml/s)
 N : (rpm)

In the case of the smallest throughput, the largest values for the backflow are calculated for the largest rotation speed due to the rotating action of the barrel. Increasing the throughput means a decrease of the backflow volume leading to a smaller slope in the graph for larger throughput.

Fig. 4. The backflow volume along 8 kneading elements, $N = 100$ rpm, $Q = 80$ ml/s, the stagger angle is 90° .

Fig. 5. The backflow volume, Q_b , as a function of the rotation speed N , for several throughputs; the stagger angle is 90° .

By comparing two cases in which $Q_1/N_1 = Q_2/N_2$, it is found that the backflow volume $|Q_{b2}|$ of the case with (N_2, Q_2) can be approximately calculated from: $|Q_{b2}| = |Q_{b1}| \cdot N_2/N_1$. This is confirmed by the similarity of the flow profiles in the down-channel direction found for the two cases.

The Transverse Velocities

In Fig. 6a the velocities in the transverse plane of the second kneading element are shown for a stagger angle of 90° , a rotation speed of 200 [rpm], and throughput 20 [ml/s]. In Fig. 6b a plane is shown that is, for the case of a stagger angle of 90° , the symmetry plane in the geometry, perpendicular to the local transverse direction. The recirculation flux for this symmetry plane, Fig. 6b, for varying stagger angle is shown in Fig. 7. In the case of a stagger angle of 90° the recirculation flux, $|Q_r|$ is practically zero, as can be seen in Fig. 6a. The recirculation flux is dependent on the stagger angle.

The Pressure Difference Over One Kneading Element

Figure 8 shows the pressure for the case of a stagger angle of 90° , averaged over the cross section, as a function of the axial coordinate z . The differences in the slope near the inflow and outflow plane are due to the influence of the blocked plane. The presence of the next element in the outflow profile causes a not completely linear pressure drop over the length of the kneading element.

The influence of rotation speed and throughput, for the pressure difference over one element, is illustrated in Fig. 9 and Eq 7. The pressure difference, ΔP , is

defined as the difference between the average pressure in the inflow plane and the outflow plane.

$$\begin{aligned} \Delta P &= c \times Q \\ \text{pressure drop/kneading element} \\ \Delta P(\text{Pa}), \quad Q(\text{m}^3/\text{s}) \\ c &= 408.5 \times 10^6 (\text{kg}/\text{m}^4\text{s}) \end{aligned} \quad (7)$$

In this expression, the constant c is dependent on the viscosity, the cross-sectional area, A , and the length of the kneading element, for $\text{Re} = 0.039$: $c = f(\eta, A^{-2}, l)$, which is confirmed by calculations, performed in the geometry of several extruders with different diameters, for which ΔP is found to scale with A^{-2} . It is interesting to note that the pressure drop, in this particular case with stagger angle 90° , is not influenced by the rotation speed. This is due to the lack of axial dragging action of the staggered elements on the fluid. In cases where the stagger angle is different from 90° , the rotational speed has been found to influence the pressure build-down.

Shear and Elongation Rate

The two components of the deformation, the shear rate $\dot{\gamma}$ and the elongation rate $\dot{\epsilon}$, are calculated. These quantities are computed with (6):

$$\begin{aligned} \dot{\epsilon} &= \frac{1}{2} (\nabla \vec{v} + \nabla \vec{v}^T) : \frac{\vec{v}}{\|\vec{v}\|} \frac{\vec{v}}{\|\vec{v}\|} \\ &= (u^2 u_x + v^2 v_y + w^2 w_z + uv(v_y + v_x) + uw(u_z + w_x) \\ &\quad + vw(v_z + w_y) / (u^2 + v^2 + w^2) \quad (8) \\ \dot{\gamma} &= \sqrt{2(\nabla \vec{v} + \nabla \vec{v}^T) : (\nabla \vec{v} + \nabla \vec{v}^T)} \\ &= ((2u_x^2 + 2v_y^2 + 2w_z^2 + (u_y + v_x)^2 \\ &\quad + (u_z + w_x)^2 + (v_z + w_y)^2)^{1/2} \end{aligned}$$

Fig. 6a. The transverse velocities, x,y-plane for the symmetrical case, $N = 200$ rpm, $Q = 5$ ml/s. Fig. 6b. The plane where the recirculation flux is calculated; the stagger angle is 90° .

The integral mean values of the rates in each cross-section of the channel, $\dot{\gamma}$ and $\dot{\epsilon}$, the integral mean values for the complete volume, $(\bar{\dot{\gamma}}, \bar{\dot{\epsilon}})$ are also calculated for various rotation speeds and throughputs (Fig. 10), in the kneading element.

The increase of shear and elongation rate due to variation of the rotation speed has two causes:

- the influence of the backflow,
- the increase in transverse velocities.

Both cause an increase in local velocity differences in the flow profile and therefore an increase in shear and in elongation rate.

For the case of a stagger angle of 90° , the following equations have been fitted for the mean shear and mean elongation rate as a function of rotation speed

and throughput.

dependence on N and Q :

$$\begin{aligned} \bar{\dot{\gamma}} &= 24.56 + 0.24 \cdot ((Q - 5)) - A_1 \times (N - 25) \\ &\quad + 0.98 \times (Q - 5) \\ A_1 &= 0.1 \times \ln(Q/5)/\ln(4) \\ \bar{\dot{\epsilon}} &= 0.0666 \times N + 0.0337 \times Q \\ N: (\text{rpm}), \quad Q: (\text{ml/s}) \end{aligned} \quad (9)$$

From Figs. 10a and b, it is clear that the rotation speed has a large effect on the shear and elongation rate. In the limit for very large rotation speeds the shear for different cases of throughput has the same value. It is concluded that in this limit the effect of the throughput on the shear rate is small compared with the effect of the rotation speed.

Fig. 7. Recirculation (ml/s) (velocities in the x,y plane) for varying stagger angle.

Fig. 8. The pressure averaged over the cross section for five axial coordinates z .

The Influence of the Stagger Angle Between the Kneading Elements on the Flow

In many geometries used in extruder technology, the kneading section is designed with several configurations. Values of 30°, 45°, and 60° for forward pitch and 120°, 135°, and 150° for backward pitch are commonly used as the stagger angles between the kneading paddles. For non-zero stagger angles, part of the outflow plane in the geometry of the kneading section is blocked.

The influence of the stagger angle on the pressure drop over one kneading element is shown in Fig. 11. In most cases the pressure drop is found to increase when the stagger angle between the kneading elements increases.

The elongation and shear rate is calculated from the flow profile for different angles between the kneading elements, Fig. 12. The size of the blocked part of the plane gradually changes with increasing angle. Since the size of this plane reaches a maximum at 90° this influences the shear and elongation rate as is visible in Fig. 12.

Dependence of the shear rate on the stagger angle,
 $90^\circ < \varphi < 150^\circ$

$$\dot{\gamma}_1 = \dot{\gamma} \cdot \exp(4.585 \times 10^{-3} \cdot \varphi) \quad (10)$$

Thus a reasonably accurate value of the shear in the case with a stagger angle larger than 90° can be calculated by using the shear ($\dot{\gamma}$) (Eq 9) in Eq 10.

Fig. 9. The pressure drop for one kneading element for varying rotation speeds and throughputs, the stagger angle is 90° .

The absolute backflow, $|Q_b|$, has a minimum in the case of a stagger angle smaller than 90° where the size of the blocked part of the outflow plane has a maximum, Fig. 13. The backflow volume is shown for varying stagger angles between the kneading elements in the case of $N = 100$ (rpm) and $Q = 80$ (ml/s). For a better understanding of the influence of the blocked part of the plane on the flow profile, the following must be kept in mind:

As mentioned, the flow profile has a large backflow volume at small or large stagger angles. Changing the stagger angle means moving the blocked part of the outflow plane from a place where a negative outflow is found to a place with a positive outflow (or vice versa). The outflow plane is blocked at the position where normally the velocities in outflow profile are negative when: $\varphi = 15^\circ, 30^\circ, 45^\circ, 60^\circ$. Using backward staggered kneading elements on the other hand, the next screw element blocks the positive outflow area, leaving room for a larger backflow to develop $\varphi = 120^\circ, 135^\circ, 150^\circ, 165^\circ$. In this case, the part of the outflow plane where the axial velocities are normally positive is blocked and a larger backflow volume develops (Fig. 13).

In Figs. 14a and b, a viscosity of 1 [Pa.s] is used, which is 100 times lower than the viscosity in Fig. 7. By comparing the transverse velocities in Fig. 14a (with a stagger angle 90°) with the transverse velocities in Fig. 14b (with a stagger angle 150°) it is clear that the flow pattern in the cross-channel direction is influenced by the stagger angle. The secondary velocities result in a transverse circulation in the "channel" of the kneading section, which was also found to increase with increasing rotation speed.

The Influence of the Viscosity on the Flow

In the case of reactive extrusion, monomer with low viscosity enters the extruder, and, upon polymerizing, the viscosity increases. For processes like this (7–10) it is of interest to calculate the flow profile for the case of a very low viscosity. In Fig. 15 relative backflow, $|Q_b^*|$, decreases as a function of the viscosity for $N = 25$ (rpm) and $Q = 20$ (ml/s) and for $N = 100$ (rpm) and $Q = 80$ (ml/s).

In Fig. 16 the influence of the viscosity on the pressure drop is linear:

$$\Delta P = 4.085 \cdot Q \cdot \eta \text{ [Pa]} \quad (11)$$

$Q(\text{ml/s}), \quad \eta(\text{Pa.s})$

With Eq 11 the pressure drop can be calculated. This may be of use in the modeling of the kneading section of reactive extrusion and mixing in corotating twin-screw extruders.

The influence of the viscosity on the shear and elongation rate in the range from 100 down to 0.01 [Pa.s] is small. At high viscosities, the convective terms in the Navier Stokes equations are small, leading to a simple Stokes flow, in which there is no more influence of viscosity. The shear rate decreases and the elongation rate increases slightly with increasing viscosity, as shown in Fig. 17. At a viscosity of 1 [Pa.s] these rates have reached their limit values corresponding to Stokes flow.

The Adiabatic Axial Temperature Rise

The viscous dissipation, due to the shear acting on the fluid, causes a temperature rise. The shear rate, as calculated, can be used to calculate the viscous dissipation for the Newtonian case. If it is assumed that no

Fig. 10. The average value over one kneading element of (a) shear and (b) elongation rate for varying rotation speed and throughput; the stagger angle is 90° .

heat leaves the extruder via the walls, and the viscous dissipation can be calculated from the average value of the shear rate, after some approximations on the heat equation, the adiabatic temperature rise is calculated with C_p ($= 2000 \text{ J/kg K}$) as the specific heat of the material. The shear rate values can be used to compute the viscous dissipation W by integration of $\eta \dot{\gamma}^2$ over the channel volume, for the Newtonian case. This leads to the following equation:

$$\Delta T = \frac{W}{Q \rho C_p} \quad (12)$$

Fig. 11. The pressure drop for different stagger angles between the kneading paddles, $N = 100 \text{ rpm}$, $Q = 80 \text{ ml/s}$.

Fig. 12. The shear and elongation rate rate for varying stagger angles, $N = 100$ rpm, $Q = 80$ ml/s.

Fig. 13. The backflow volume for different stagger angles between succeeding kneading paddles, $N = 100$ rpm, $Q = 80$ ml/s.

In Fig. 18 the temperature rise ($^{\circ}\text{C}$) over one single kneading element is shown as a function of the rotation speed for varying throughputs. The temperature increase over one short kneading element is small because the viscosity chosen here is 100 [Pa.s], which is a relative small value.

Experimental Validation

The pressure drop as calculated in Eq 7 is measured in an intermeshing corotating twin-screw extruder. The experimental setup is described in Ref. 9, and the experiments are done with polystyrene (Shell, PS 7000), seven kneading elements, and a barrel temperature of 200°C . For all throughputs the viscosity was calculated to be close to 180 Pas at the rotation speed, throughput, and temperature (measured with an IR thermometer) in the kneading section.

The computed pressure drop is shown in Fig. 19 to be comparable with the measured values, within the experimental error of 5%. The temperature rise, due to the viscous dissipation, is calculated in Ref. 9 with the

Fig. 14. The transverse velocities for two cases of the stagger angle (at five axial positions), (a): angle: 90° , (b): angle: 150° ; both $N = 100$ rpm, $Q = 80$ ml/s.)

Fig. 15. The relative backflow volume for varying viscosities, $N = 100$ rpm, $Q = 80$ ml/s, the stagger angle is 90° .

Fig. 16. The pressure drop for varying viscosities, $N = 100$ rpm, $Q = 80$ ml/s, the stagger angle is 90° .

results for shear rate given under **Shear and Elongation Rate**. Since in Ref. 9 it is found that the calculated temperature rise due to the shear is comparable with measured values, within the experimental error (10%) it can be concluded that our results for shear rate also reasonable.

DISCUSSION AND CONCLUSIONS

The results of this paper and the companion paper (11) can be used when designing screw geometries in corotating twin-screw extruders for the processing of polymers. The pressure gradient in the kneading elements is found to be independent of the rotation speed only for a stagger angle of 90° . For other stagger angles, pressure drop is influenced by rotational speed, as is also the case for the transporting element, as calculated in Ref. 11. In the transporting element the pressure gradient is found to be dependent on the rotation speed. The completely filled length in the transporting element can be found by using the pressure gradient, $\partial P / \partial z$, in (11), and is calculated from the ratio of the

(a)

(b)

Fig. 17. The (a) shear and (b) elongation rate for varying viscosities, $N = 100$ rpm, $Q = 80$ ml/s.

pressure drop in the kneading section and the pressure buildup in the transporting section:

$$(\Delta P(Q, N), kn) / \left(\frac{\partial}{\partial z} P(Q, N), tr \right)$$

A number of conclusions can be drawn from our results:

- The average values of shear and elongation rate in kneading elements depend strongly on processing parameters. Since mixing is dependent on the shear and elongation rate (9), the results presented in this paper can be used when two polymers are mixed in a corotating twin-screw extruder.
- The shear rate is found to be much larger than the elongation rate, even in the kneading section.
- The ratio between the pressure drop and the viscosity is constant.

Fig. 18. The adiabatic temperature increase as a function of rotation speed, N for several throughputs.

Fig. 19. The measured and calculated pressure drop over one kneading element as a function of the throughput.

- The graphs and equations found can be used in other computer calculations to find parameters of interest, such as distribution in residence times (12) and axial temperature profiles, in the kneading section. It must be kept in mind, however, that this is valid only within the limitations of these calculations. A larger backflow volume will lead to a larger residence time distribution. Variation of the backflow is found when the throughput or rotation speed is varied.
- In the case of reactive extrusion or reactive compounding the expressions found can be used in modeling of parameters, such as the pressure drop, to confirm experimental trends.

The results in Ref. 13 show the resemblances and differences between transporting and kneading elements. Here we find that the drop of pressure in the 90° kneading elements is independent of N , and for the transporting elements, it is found that the influence of N is prominent. Consequently, the length required for the buildup of pressure (and, so the residence time distribution) can be modified by changing N , which will not influence the drop of pressure in the kneading elements with a stagger angle of 90°. A comparison of the shear and elongation rates with the kneading (stagger angle: 90°), shows that the difference between the two kinds of elements increases with Q . This difference increases when the kneading elements are backward. In reality, this difference could be larger because the transporting elements are not

always completely filled and also because the intermeshing area from the two kneading elements is not used in the modeling from Ref. 9. The influence of the viscosity on the axial gradient of pressure is important ($\Delta P/\eta = \text{constant}$ is found) and is similar for the kneading elements. As for the kneading elements, the variation of the parameters studied, with the viscosity, is faster for a larger rotation speed.

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NOMENCLATURE

- A (m²) = Area through which the fluid in the kneading section flows.
 A_i = Fitted parameter.
 C_l (m) = Centerline distance of the twin-screw extruder.
 h (m) = Channel depth without clearance.
 L = Divergence matrix.
 l (m) = Length of one kneading element (14 mm).
 M_p = Pressure mass matrix.
 n (—) = Number of screw threads.
 N (rpm) = Rotation speed.
 $N(\vec{u})\vec{u}$ = Discretization of the convective terms.
 p (Pa) = Vector of pressures unknowns.
 P (Pa) = Pressure.
 ΔP (Pa/mm) = Pressure drop over one kneading element.
 $\Delta P(Q, N, \text{kn})$ = Pressure consumed in one kneading element.
 $(\partial/\partial z)P(N, Q)$ = Pressure gradient in the transportation element, Part I.
 τ (Pa/mm) = Stagger angle between the kneading paddles.
 φ (degree) = Stagger angle between the kneading paddles.
 Q (ml/s) = Throughput of the extruder.
 Q_B (ml/s) = Integral of the axial negative flow volume, also called backflow volume, on a cross section.
 $Q_B^*(-) Q_B/Q$ = Relative backflow volume, on a cross section.
 Q_r (ml/s) = Recirculation flux.
 R_s (m) = Radius of the screw.
 Re (—) = Reynolds number $Re = \rho v d/\eta$.
 S = Stress matrix.
 dT (°C) = Temperature rise per kneading element, $\eta = 180$ (Pa.s).
 $\vec{v}$ (m/s) = Velocity vector (with components u, v, w).

- W (m) = Width of the kneading paddle.
 x, y (m) = Transverse coordinates.
 z (m) = Axial coordinate.
 $\dot{\gamma}$ (s^{-1}) = Local shear rate.
 $\dot{\epsilon}$ (s^{-1}) = Local elongation rate.
 $\bar{\dot{\gamma}}$ (s^{-1}) = Shear rate averaged over the volume, Eq 9.
 $\bar{\dot{\epsilon}}$ (s^{-1}) = Elongation rate averaged over the volume, Eq 9.
 σ (s^{-1}) = Stress.
 η (Pas) = Viscosity.
 ρ (kg/m^3) = Density of the fluid.

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